Lefschetz-thimble path integral for studying the Silver Blaze problem

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Motivation: Sign problem, Silver Blaze problem

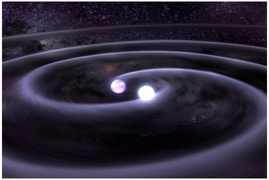
Sign problem of finite-density QCD

QCD

Fundamental theory for quarks and gluons

Neutron star

- Cold and dense nuclear matter
- $2m_{\rm sun}$ neutron star (2010)
- Gravitational-wave observations (2016$\sim$)



Neutron star merger

(image from NASA)

Reliable theoretical approach to equation of state must be developed!

$$Z_{\rm QCD}(T,\mu)=\int \mathcal{D}A\, \underbrace{\mathrm{Det}(\not{D}(A,\mu_q)+m)}_{\rm quark}\underbrace{\exp\left(-S_{\rm YM}(A)\right)}_{\rm gluon}.$$

Sign problem: $\mathrm{Det}(\not{D}(A,\mu_q)+m)\not\geq 0$ at $\mu_q\neq 0$.

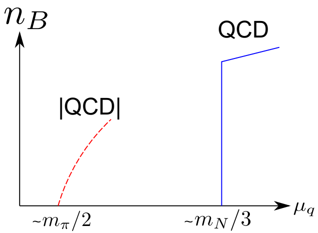
Sign problem of finite-density QCD

QCD & |QCD|

$$Z_{\mathrm{QCD}} = \int \mathcal{D}A \, (\det \not{D}) \, \mathrm{e}^{-S_{\mathrm{YM}}}, \; Z_{|\mathrm{QCD}|} = \int \mathcal{D}A \, |\det \not{D}| \, \mathrm{e}^{-S_{\mathrm{YM}}}.$$

If these two were sufficiently similar, we have no practical problems. However, it was observed in lattice QCD simulation that at $T=0$

(e.g., Barbour et. al. (PRD **56** (1998) 7063))



Baryon Silver Blaze problem

The curious incident of the dog in the night-time (Holmes, Silver Blaze).

Problem: Show that $n_B = 0$ for $\mu_q < m_N/3$ using path integral.
(Cohen, PRL **91** (2003) 222001)

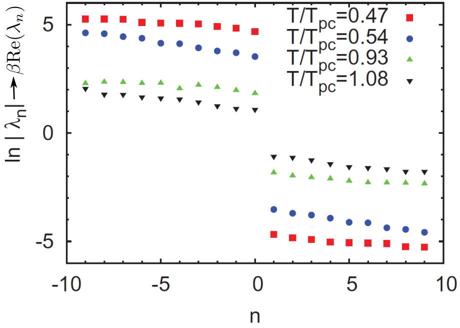
Current situation: For $\mu_q < m_\pi/2$, the problem is solved.
Quark det. is

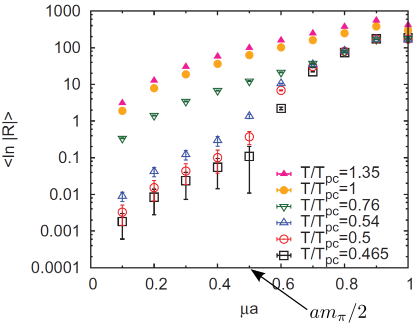
$$\frac{\mathrm{Det}(\not{D}(A,\mu_q)+m)}{\mathrm{Det}(\not{D}(A,0)+m)} \simeq \prod_{0<\mathrm{Re}(\lambda_A)<\mu_q} \left(1+\mathrm{e}^{-\beta(\lambda_A-\mu_q)}\right),$$

and $\text{ess-min}_A(\mathrm{Re}(\lambda_A)) = m_\pi/2$. (Cohen, PRL **91** (2003) 222001, Adams, PRD **70** (2004) 045002, Nagata et. al., PTEP **2012** 01A103).

Spectrum of $\gamma_4(\not{D}_A + m)$

Gap of $\{\lambda_n\}_n = \mathrm{Spec}\{\gamma_4(\not{D}_A + m)\}$ gives the pion mass (Gibbs).





Lattice study of the quark spectrum and the Dirac determinant.

(Nagata et. al., PTEP **2012** 01A103)

Method: Path integral on Lefschetz thimbles

Sign problem of path integrals

Consider the path integral:

$$Z = \int \mathcal{D}x \exp(-S[x]).$$

- $S[x]$ is real $\Rightarrow$ No sign problem. Monte Carlo works.
- $S[x]$ is complex $\Rightarrow$ Sign problem appears!

If $S[x] \in \mathbb{C}$, eom $S'[x] = 0$ may have no real solutions $x(t) \in \mathbb{R}$.

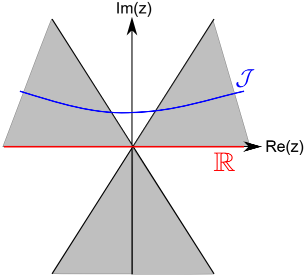
Idea: Complexify $x(t) \in \mathbb{C}$!

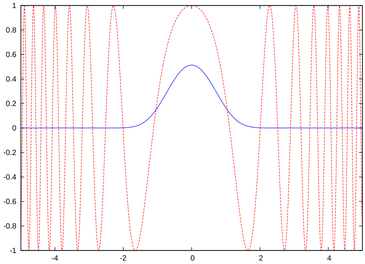
Lefschetz thimble for Airy integral

Airy integral is given as

$$\mathrm{Ai}(a) = \int_{\mathbb{R}} \frac{\mathrm{d}x}{2\pi} \exp \mathrm{i} \left(\frac{x^3}{3} + ax \right)$$

Complexify the integration variable: $z = x + \mathrm{i}y$.





Integrand on $\mathbb{R}$, and on $\mathcal{J}_1$ $(a = 1)$

Rewrite the Airy integral

There exists two Lefschetz thimbles $\mathcal{J}_\sigma$ $(\sigma = 1, 2)$ for the Airy integral:

$$\mathrm{Ai}(a) = \sum_\sigma n_\sigma \int_{\mathcal{J}_\sigma} \frac{\mathrm{d}z}{2\pi} \exp \mathrm{i} \left(\frac{z^3}{3} + az \right).$$

n_σ: intersection number of the steepest ascent contour $\mathcal{K}_\sigma$ and $\mathbb{R}$.

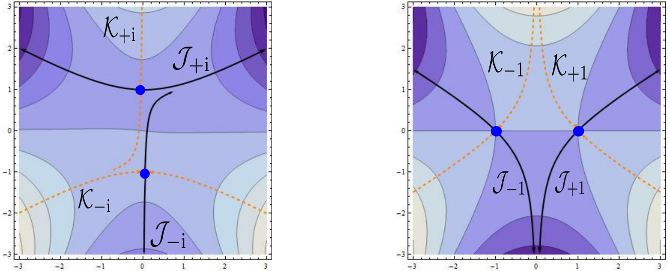


Figure: Lefschetz thimbles $\mathcal{J}$ and duals $\mathcal{K}$ $(a = 1\mathrm{e}^{0.1\mathrm{i}}, -1)$

Lefschetz decomposition formula

Oscillatory integrals with **many variables** can be evaluated using the "steepest descent" cycles $\mathcal{J}_\sigma$: (classical eom $S'(z_\sigma)=0$)

$$\int_{\mathbb{R}^n} \mathrm{d}^n x\, \mathrm{e}^{-S(x)} = \sum_\sigma \langle \mathcal{K}_\sigma, \mathbb{R}\rangle \int_{\mathcal{J}_\sigma} \mathrm{d}^n z\, \mathrm{e}^{-S(z)}.$$

$\mathcal{J}_\sigma$ are called Lefschetz thimbles, and $\mathrm{Im}[S]$ is constant on it:

$$\mathcal{J}_\sigma = \left\{ z(0) \middle| \lim_{t\to-\infty} z(t) = z_\sigma \right\}, \quad \frac{\mathrm{d}z^i(t)}{\mathrm{d}t} = \overline{\left(\frac{\partial S(z)}{\partial z^i}\right)}.$$

$\langle \mathcal{K}_\sigma, \mathbb{R}\rangle$: intersection numbers of duals $\mathcal{K}_\sigma$ and $\mathbb{R}^n$ $(\mathcal{K}_\sigma = \{z(0) | z(\infty) = z_\sigma\})$.

[Witten, arXiv:1001.2933, 1009.6032]

[Christoforetti et al. (PRD(2012)), Fujii et al. (JHEP 1310), etc.]

Analysis: Semi-classical analysis of the one-site Hubbard model

One-site Fermi Hubbard model

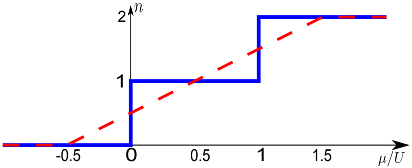
One-site Hubbard model:

$$\hat{H} = U\hat{n}_\uparrow \hat{n}_\downarrow - \mu(\hat{n}_\uparrow + \hat{n}_\downarrow).$$

Fock state gives the number density immediately:

$$\langle \hat{n} \rangle = \frac{1}{\beta}\frac{\partial}{\partial \mu}\ln Z = \frac{2(\mathrm{e}^{\beta\mu} + \mathrm{e}^{\beta(2\mu - U)})}{1 + 2\mathrm{e}^{\beta\mu} + \mathrm{e}^{\beta(2\mu-U)}}.$$

In the zero-temperature limit,



(YT, Hidaka, Hayata, 1509.07146)(cf. Monte Carlo with 1-thimble approx. gives a wrong result: Fujii, Kamata, Kikukawa,1509.08176, 1509.09141; Alexandru, Basar, Bedaque,1510.03258.)

Path integral for one-site model

Effective Lagrangian of the one-site Hubbard model:

$$\mathcal{L} = \frac{\phi^2(\tau)}{2U} + \psi^* \left[\partial_\tau - (U/2 + \mathrm{i}\phi(\tau) + \mu)\right] \psi.$$

The path-integral expression is ($\varphi = \int_0^\beta \phi(\tau)\mathrm{d}\tau/\beta$)

$$Z = \sqrt{\frac{\beta}{2\pi U}} \int_{\mathbb{R}} \mathrm{d}\varphi \underbrace{\left(1 + \mathrm{e}^{\beta(\mathrm{i}\varphi + \mu + U/2)}\right)^2}_{\text{Fermion Det}} \mathrm{e}^{-\beta\varphi^2/2U}.$$

Integrand has complex phases causing the sign problem.

φ is an auxiliary field for the number density:

$$\langle \hat{n} \rangle = \mathrm{Im}\langle \varphi \rangle / U.$$

Sign problem and fermion determinant

One-site Hubbard model:

$$\mathrm{Det}\left[\partial_\tau - \left(\mu + \frac{U}{2} + \mathrm{i}\varphi\right)\right] = \left(1 + \mathrm{e}^{-\beta(-U/2-\mu)}\mathrm{e}^{\mathrm{i}\beta\varphi}\right)^2 .$$

Quark determinant in QCD:

$$\mathrm{Det}\left[\gamma_4(\not{D}_A + m) - \mu\right] = \mathcal{N}(A)\prod_{\varepsilon_j>0}(1+\mathrm{e}^{-\beta(\varepsilon_j-\mu-\mathrm{i}\phi_j)})(1+\mathrm{e}^{-\beta(\varepsilon_j+\mu+\mathrm{i}\phi_j)}),$$

where the spectrum of $\gamma_4(\not{D}_A + m)$ is

$$\lambda_{(j,n)} = \varepsilon_j(A) - \mathrm{i}\phi_j(A) + (2n+1)\mathrm{i}\pi T.$$

Minimal value of $\varepsilon(A) = m_\pi/2$.

Silver Blaze problem for $\mu < -U/2$, $\mu < m_\pi/2$

One-site Hubbard model: As $\beta U \gg 1$ and $-U/2 - \mu > 0$,

$$\mathrm{Det}\left[\partial_\tau - \left(\mu + \frac{U}{2} + \mathrm{i}\varphi\right)\right] = \left(1 + \mathrm{e}^{-\beta(-U/2-\mu)}\mathrm{e}^{\mathrm{i}\beta\varphi}\right)^2 \simeq 1.$$

The sign problem almost disappears, so that $\mathcal{J}_* \simeq \mathbb{R}$.

Finite-density QCD: As $\beta \to \infty$ and $\mu < m_\pi/2$,

$$\frac{\mathrm{Det}\left[\gamma_4(\not{D}_A + m) - \mu\right]}{\mathrm{Det}\left[\gamma_4(\not{D}_A + m)\right]} \to 1.$$

The sign problem disappears by the reweighting method.

$\Rightarrow$ Lefschetz thimbles $\simeq$ Original integration regions

Flows at $\mu/U < -0.5$ (and $\mu/U > 1/5$)

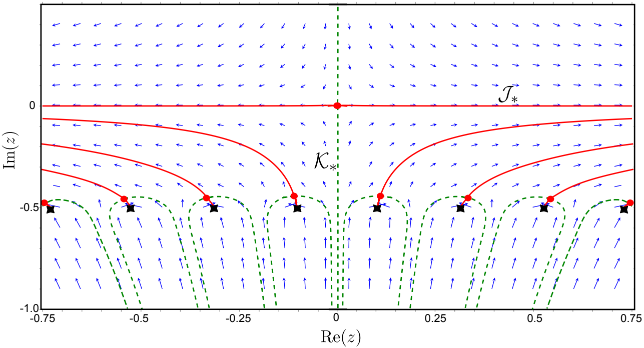


Figure: Flow at $\mu/U = -1$. $\mathcal{J}_* \simeq \mathbb{R}$.

$$Z = \int_{\mathcal{J}_*} \mathrm{d}z \, \mathrm{e}^{-S(z)}.$$

Number density: $n_* = 0$ for $\mu/U < -0.5$, $n_* = 2$ for $\mu/U > 1.5$.

(YT, Hidaka, Hayata, 1509.07146)

Silver Blaze problem for $\mu > -U/2$, $\mu > m_\pi/2$

One-site Hubbard model: At each real config., the magnitude is exponentially large:

$$\mathrm{Det}\left[\partial_\tau - \left(\mu + \frac{U}{2} + \mathrm{i}\varphi\right)\right] = O\left(\mathrm{e}^{\beta(U+\mu/2)}\right)$$

This large contributions must be canceled exactly in order for $n = 0$.

Finite density QCD: The situation is almost the same, since

$$\frac{\mathrm{Det}(\not{D}(A,\mu_q)+m)}{\mathrm{Det}(\not{D}(A,0)+m)} \simeq \prod_{\mathrm{Re}(\lambda_A)<\mu_q} \exp\beta\left(\mu_q - \lambda_A\right),$$

but $n_B = 0$ for $\mu_q \lesssim m_N/3$.

Flows at $-0.5 < \mu/U < 1.5$

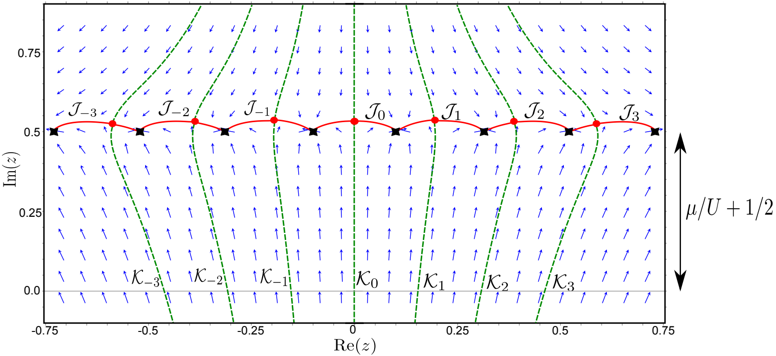


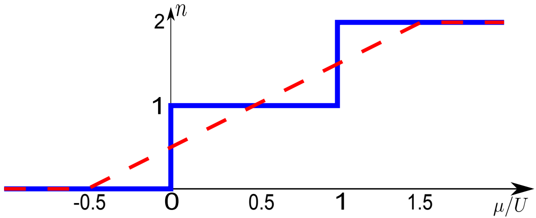
Figure: Flow at $\mu/U = 0$

Complex saddle points lie on $\mathrm{Im}(z_m)/U \simeq \mu/U + 1/2$.

This value is far away from $n = \mathrm{Im}\langle z \rangle/U$=0, 1, or 2.

Curious incident of n in one-site Hubbard model

We have a big difference bet. the exact result and naive expectation:

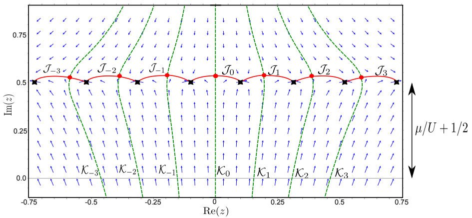


This is similar to what happens for QCD and |QCD|.
$\mu/U = -0.5 \Leftrightarrow \mu_q = m_\pi/2$.

Complex classical solutions

If $\beta U \gg 1$, the classical sol. for $-0.5 < \mu/U < 1.5$ are labeled by $m \in \mathbb{Z}$:

$$z_m \simeq \mathrm{i}\left(\mu + \frac{U}{2}\right) + 2\pi m T.$$



At these solutions, the classical actions become

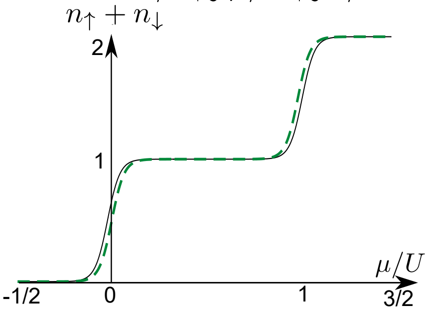
$$S_0 \simeq -\frac{\beta U}{2}\left(\frac{\mu}{U}+\frac{1}{2}\right)^2,$$
$$\mathrm{Re}\,(S_m - S_0) \simeq \frac{2\pi^2}{\beta U} m^2,$$
$$\mathrm{Im}\, S_m \simeq 2\pi m \left(\frac{\mu}{U}+\frac{1}{2}\right).$$

Semiclassical partition function

Using complex classical solutions z_m, let us calculate

$$Z_{\mathrm{cl}} := \sum_{m=-\infty}^{\infty} \mathrm{e}^{-S_m} = \mathrm{e}^{-S_0(\mu)} \theta_3 \left(\pi \left(\frac{\mu}{U} + \frac{1}{2} \right), \mathrm{e}^{-2\pi^2/\beta U} \right).$$

This expression is valid for $-1/2 \lesssim \mu/U \lesssim 3/2$.



Important interference among multiple thimbles

Let us consider a "phase-quenched" multi-thimble approximation:

$$Z_{|\mathrm{cl.}|} = \sum_m \left|\mathrm{e}^{-S_m}\right| = \mathrm{e}^{-S_0(\mu)}\theta_3(0, \mathrm{e}^{-2\pi^2/\beta U}).$$

- Lee–Yang zeros cannot appear at $\mu/U = 0,\, 1$.
- One-thimble, or "phase-quenched", result: $n \simeq \mu/U + 1/2$.

Consequence

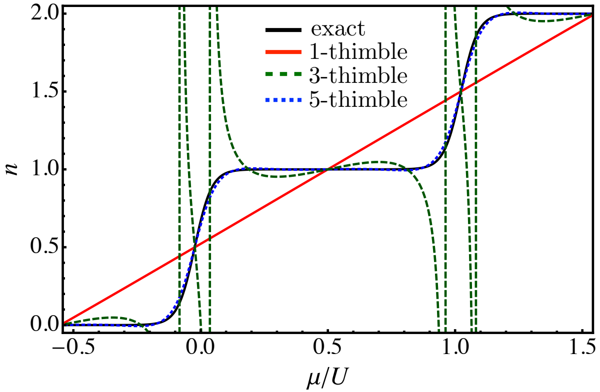
To understand the Silver Blaze problem, we need interference of complex phases among different Lefschetz thimbles.

(cf. Particle Productions: Dumulu, Dunne, PRL 104 250402)

(cf. Hidden Topological Angles: Behtash, Sulejmanpasic, Schäfer, Ünsal, PRL 115 041601)

Numerical results

Results for $\beta U = 30$: (1, 3, 5-thimble approx.: $\mathcal{J}_0$, $\mathcal{J}_0 \cup \mathcal{J}_{\pm 1}$, and $\mathcal{J}_0 \cup \mathcal{J}_{\pm 1} \cup \mathcal{J}_{\pm 2}$)



Necessary number of Lefschetz thimbles $\simeq \beta U/(2\pi)$.

(YT, Hidaka, Hayata, NJP 18 (2016) 033002, arXiv:1509.07146[hep-th])

Bonus: Complex Langevin method

Complex Langevin method

Complex Langevin has been regarded as a sign-problem solver via stochastic quantization (Klauder, PRA 29, 2036 (1984), Parisi, PLB 131, 393 (1983)):

$$\frac{\mathrm{d}z_\eta(\theta)}{\mathrm{d}\theta} = -\frac{\partial S}{\partial z}(z_\eta(\theta)) + \sqrt{\hbar}\eta(\theta).$$

θ: Stochastic time, η: Random force $\langle \eta(\theta)\eta(\theta')\rangle_\eta = 2\delta(\theta-\theta')$.

Properties:

- Numerical cost is very cheap.
- Ito calculus shows $\langle O(z_\eta(\infty))\rangle_\eta$ solve the Dyson–Schwinger eq.
- Sign problem does not appear.
- But, it fails in some cases. $\Rightarrow$ When does it fail?

Semiclassical incorrectness of CL method

If $\hbar$ is small enough, we can show a sufficient condition for incorrect behaviors of CL method.

(Hayata, Hidaka, YT, 1511.02437)

Since $\hbar \ll 1$, CL distribution would accumulate around $\{z_\sigma\}$:

$$^{\exists}c_\sigma \geq 0 \quad \text{s.t.} \quad \langle O(z_\eta)\rangle_\eta \simeq \sum_\sigma c_\sigma O(z_\sigma).$$

Assume for contradiction that CL method is correct, then

$$\begin{aligned}\langle O(z_\eta)\rangle_\eta &\overset{!}{=} \int_{\mathbb{R}} \mathrm{d}x \mathrm{e}^{-S(x)/\hbar} O(x) \\ &= \frac{1}{Z}\sum_\sigma \langle \mathcal{K}_\sigma, \mathbb{R}^n\rangle \int_{\mathcal{J}_\sigma} \mathrm{d}z\, \mathrm{e}^{-S(z)/\hbar} O(z).\end{aligned}$$

Semiclassical inconsistency

In the semiclassical analysis, one now obtains (for dominant saddle points)

$$c_\sigma = \frac{\langle \mathcal{K}_\sigma, \mathbb{R}^n \rangle}{Z} \sqrt{\frac{2\pi\hbar}{S''(z_\sigma)}} \mathrm{e}^{-S(z_\sigma)/\hbar}.$$

The right hand side can be complex, which contradicts with $c_\sigma \geq 0$!
(Hayata, Hidaka, YT, 1511.02437)

We show that the complex Langevin is wrong if

- There exist several dominantly contributing saddle points, and
- Those saddle points have different complex phases.

Proposal for modification

Assume as a working hypothesis that

$$c_\sigma = \frac{\langle \mathcal{K}_\sigma, \mathbb{R} \rangle}{Z} \left| \sqrt{\frac{2\pi\hbar}{S''(z_\sigma)}} \mathrm{e}^{-S(z_\sigma)/\hbar} \right|.$$

Because of the localization of probability distribution P, it would be given as

$$P = \sum_\sigma c_\sigma P_\sigma, \quad \mathrm{supp}(P_\sigma) \cap \mathrm{supp}(P_\tau) = \emptyset.$$

Assumption means "CL = phase quenched multi-thimble approx.":

$$\langle O(z_\eta) \rangle_\eta \simeq \sum_\sigma \frac{\langle \mathcal{K}_\sigma, \mathbb{R} \rangle}{Z} \left| \sqrt{\frac{2\pi\hbar}{S''(z_\sigma)}} \mathrm{e}^{-S(z_\sigma)/\hbar} \right| O(z_\sigma).$$

Proposal for modification (conti.)

If so, defining the phase function

$$\Phi(z,\overline{z})=\sum_{\sigma}\sqrt{\frac{|S''(z_\sigma)|}{S''(z_\sigma)}}\mathrm{e}^{-\mathrm{i}\,\mathrm{Im}\,S(z_\sigma)/\hbar}\chi_{\mathrm{supp}(\mathrm{P}_\sigma)}(z,\overline{z}),$$

we can compute

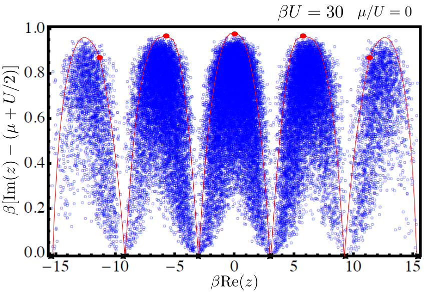
$$\langle O(z_\eta)\rangle^{\mathrm{new}}:=\frac{\langle\Phi(z_\eta,\overline{z}_\eta)O(z_\eta)\rangle_\eta}{\langle\Phi(z_\eta,\overline{z}_\eta)\rangle_\eta}.$$

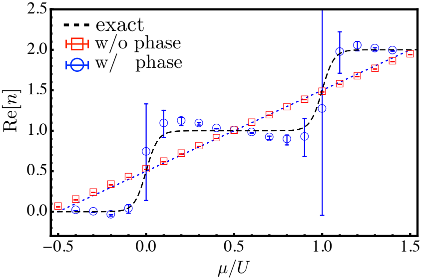
This new one is now consistent within the semiclassical analysis.

(Hayata, Hidaka, YT, arXiv:1511.02437[hep-lat])

Caution: Our proposal evades inconsistency, but is not necessarily correct. Can we improve the proposal?

Complex Langevin study of one-site fermion model





(Hayata, Hidaka, YT, 1511.02437)

Complex Langevin method cannot study the Silver Blaze problem of this model without introducing the reweighting procedure.

Summary and Conclusion

- Picard–Lefschetz theory gives a suitable framework for saddle-point analysis even if $S(\phi)$ takes complex values.
- One-site Hubbard model is a nice toy model to play with the sign problem.
- Destructive and constructive interference of complex phases among Lefschetz thimbles play a pivotal role for the baryon Silver Blaze.